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ENOSE Performance in Transient Time and Steady State Area of Gas Sensor Response for Ammonia Gas: Comparison and Study

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ABSTRACT

This paper proposed an electronic nose system that utilized a SnO_2 semiconductor sensor array to detect volatile ammonia gas in farmland. All sensors were controlled by the Arduino development board. The system could collect data during both the steady-state and transient phases of sensor operation. The collected data was analyzed using PCA (principal component analysis) and MLP (Multi-layer perceptron) neural networks. The experiment was divided into two parts: The first part analyzed four concentrations of ammonia (100ppm, 200ppm, 400ppm, and Air) using PCA and MLP, which successfully distinguished the concentrations with an identification rate of over 95%. In the second part, four gases (air mixed with ammonia, pure ammonia gas, air mixed with ethanol, and pure ethanol) were analyzed using PCA and MLP, with the electronic nose system successfully distinguishing between the four types of gases. The system could read and process data during the transient phase of the sensor, and the constructed sensor array electronic nose system and acquisition method has significant potential for ammonia detection in agricultural environments.

CCS CONCEPTS

• **Computing methodologies**; • **Machine learning**; • **Machine learning approaches**; • **Neural networks**;

KEYWORDS

Electronic nose, Volatile ammonia, PCA, MLP, Neural network

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1 INTRODUCTION

Ammonia (NH_3) is a colorless gas known for its pungent odour, which poses a serious threat to human and animal health and the environment. When exposed to moist mucous surfaces such as those found in the respiratory tract, skin, and eyes, ammonia reacts to form a corrosive alkaline solution (ammonium hydroxide), leading to liquefaction necrosis [1]. Inhaling ammonia can cause damage to airways and, in extreme cases, even result in acute death [2]. In pigs, ammonia exposure can trigger lung damage and inflammation, which can adversely affect meat quality [3]. Furthermore, ammonia emissions have been linked to an increase in PM2.5 concentrations in the air [4], a type of atmospheric particulate matter that poses significant health risks, including the potential for severe illness and death. With modern industrial advancements, producing ammonia has become more cost-effective. Ammonia is widely used as a nitrogen fertilizer in agriculture, but the use of such fertilizers can lead to increased ammonia emissions into the atmosphere [5]. Research from years ago suggests that the majority of atmospheric ammonia is attributed to agriculture, accounting for 55% of emissions. In China, 29% of ammonia emissions come from livestock and 47% from agricultural fertilizer usage [6]. Therefore, detecting volatile ammonia levels in farmland is critical for managing and mitigating environmental pollution caused by agriculture. The ammonia can be detected over various methods as follows:

The electrochemical method involves an ammonia sensor capable of detecting gas concentrations as low as 1 ppm. Different materials adsorb NH_3, leading to changes in electrical signals such as resistance, voltage, and current. These alterations allow for the calculation of ammonia concentration [7, 8].

The chemiluminescence method offers a detection range of 0.25-100ppm for ammonia gas at the ppb level, making it suitable for field detection. Notably, this method boasts a fast response speed. Hu, et al. [9] have devised a catalytic luminescent gas sensor that accurately measures the ammonia concentration by analyzing the light emitted through the reaction between the gas and the catalyst surface [7]. **The passive collector method** involving the collection of gas via a membrane can accurately measure ammonia volatilization levels within a range of 0.2 ppb to 100 ppb for up to a month [7]. However, it has a drawback in that it necessitates frequent manual replacement of collection materials, resulting in excessive consumption of manpower and material resources in monitoring large areas. Additionally, the method does not provide real-time measurements of ammonia concentration, as the collected materials must be analyzed to determine the concentration of ammonia. **The photoacoustic method** is an accurate way to detect ammonia concentrations ranging from 0.3-10ppm in a laboratory setting. Laser radiation, modulated in either frequency or amplitude, is absorbed in wavelengths that align with the absorption characteristics of the target substance. This produces sound waves that can be monitored with minimal noise [10]. Though the photoacoustic method is resistant to environmental interference, it necessitates expensive and cumbersome optical equipment, which renders it unsuitable for large-scale ammonia detection in agriculture. **The fluorescence method** can detect ammonia ranging from 0.5-50ppm in the laboratory. Zhang and Lim [11]created a colorimetric array comprising 4×4 dyes using fluorescence technology to analyze the medium's color before and after exposure to gas and determine ammonia concentration. However, this method is time-consuming and unsuitable for detecting ammonia concentration in agricultural environments. But over than mentioned methods, enose over its benefit attracts more researchers. Electronic noses have several benefits for gas ammonia detection, including their ability to detect low levels of ammonia, their fast response time, and their cost-effectiveness compared to traditional methods of ammonia detection [12]. To analyze the enose data various methods were implemented but the most common can be named PCA, Artificial Neural Networks (ANNs), Support Vector Machines (SVMs) [13], Partial Least Squares (PLS), and Fuzzy Logic [12]. This paper proposes an electronic nose sensor array system for the detection of volatile ammonia in farmland. The system employs PCA and MLP to differentiate between various gases and varying concentrations of ammonia. The research contribution can be listed below: 1) Proposed an electronic nose system that utilizes a SnO_2 semiconductor sensor array for detecting volatile ammonia gas in various concentrations. 2) Collected data during both the steady-state and transient time of sensor operation and show the transient time area ability for gas concentration detection. 3) Analyzed the collected data using PCA and MLP neural networks and successfully distinguished between four concentrations of ammonia (100ppm, 200ppm, 400ppm, and Air) with an identification rate of over 95% using PCA and MLP. 4) Distinguished between four types of gases, including Air mixed with ammonia and pure ammonia gas, using PCA and MLP. 5) Demonstrated the system's ability to read and process data during the transient area of the sensor. The paper is organized as follows: The first section covers the gas sensor array, chamber structure, and data acquisition, while section III delves into the data processing methodology. In section IV, the paper concludes by analyzing and contrasting the results obtained in two modes: identifying different concentrations of ammonia and distinguishing between various odours.

2 MATERIALS AND METHODS

2.1 Gas Sensor Array

To experiment, a sensor array was created using seven different models of TGS and MQ semiconductor sensors as shown in Table 1 All sensors are controlled by the Arduino-Mega development board, Arduino is easier to control and use than other microcontrollers and can monitor sensor data directly from the IDE (Integrated development environment.

As it is shown in Table 1 the sensor array can sense the various PPM amount of VOC. In comparison to other types of gas sensors, the SnO_2 metal oxide semiconductor gas sensor offers low production cost, a simple manufacturing process, and high sensitivity [14]. However, the MQ series sensors are sensitive to changes in moisture, temperature, and humidity, which can affect sensor response. To maintain consistency in the test results, the experiment strictly controlled environmental temperature and humidity.

2.2 Chamber structure and Data Acquisition

The data acquisition system utilized in this research is the system proposed in our previous paper [15]. This system incorporates a sensor array consisting of the gas sensors listed in Table 1. To measure temperature, the LM35 sensor is utilized, while the SHT11 sensor is employed for measuring temperature and humidity. In addition to these sensors, the system also incorporates an Aquarium Air pump, power supply, and DC fan, as shown in Figure 1 (a). As the figure depicted, the sampling chamber is comprised of a 31cm high and 5cm diameter cylinder, fitted with a DC fan at one end and an electronic PCB containing a sensor array at the other. A syringe for sample and air input is connected to the wall of the chamber, with a paper towel substrate placed at the bottom to collect ammonia liquid samples and allow for evaporation. The ambient temperature and relative humidity are detected by an SHT11 sensor and LM35. Then in order to volatilize ammonia gas in the sampling room, ammonia with a known concentration is injected into the sample syringe and then into the tissue in the sampling chamber, causing the liquid to evaporate and form ammonia gas. The sensors data in the next step sensor data acquired with the help of Arduino Mega and stored in a Personal computer (PC) followed to have some advantages like flexibility, low cost, ability to connect and communicate with external parts such as sensors, etc monitors, no need for additional software or other compilers with a simple software environment. The proposed enose assembly utilizes an aquarium pump to deliver fresh air and maintain a clean sampling chamber. The pump has a compact size of 98×66×20mm and requires only 4W of power. Additionally, a DC electric fan with dimensions of 10×10cm and a voltage of 12v has been chosen to

Table 1: The sensor parameters used in the experiment

Sensor	Main sensing gas	Measurement range
MQ2	LPG, propane, methane, hydrogen, carbon monoxide, and alcohol	300-10000ppm
MQ3	Ethanol Vapor	10-1000ppm
MQ5	LPG, propane, hydrogen, methane, and other combustible gases	300-10000ppm
MQ6	LPG, butane, propane, methane, alcohol, hydrogen, and smoke	300-10000ppm
MQ7	Carbon Monoxide	10-1000ppm
MQ137	Ammonia	5-200 ppm.
TGS813	Methane, Propane, Butane	500-10000ppm

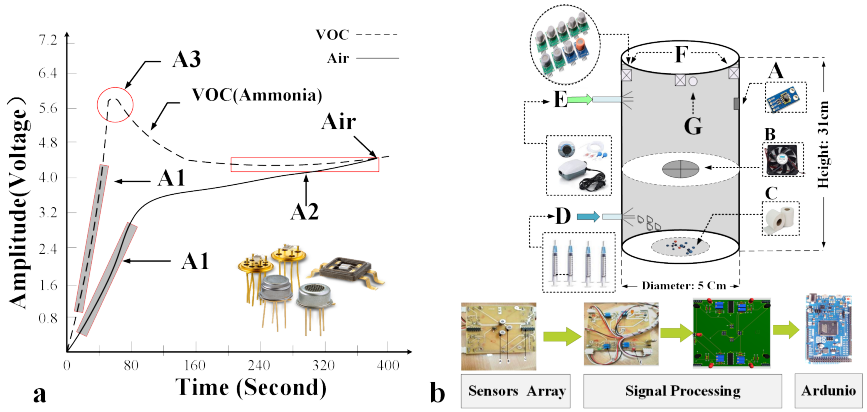

Figure 1: a: The second-order response curve of the sensor (TGS and MQ gas sensors) A1: The transient ascending stage A2: The overshoot stage A3: The steady-state stage; b: Electronic nose sensor array data sampling system A: Temperature/Humidity sensor (SHT11) B: DC fan C: Tissue paper. D: Injection syringe E: Inlet fresh air by Aquarium pump

expedite the cleaning process of the chamber. This fan will further enhance the efficiency of the enose assembly [16]. In order to calculate the ammonia concentration Equation 1) proposed by Wang, et al. [17] was used.

$$C = \frac{22.4\rho TV_s}{273MV} \times 1000 \quad (1)$$

Equation 1) relates the concentration of ammonia in parts per million (ppm), denoted by C, to the density of ammonia (ρ, measured in g·mL^{-1}), the temperature inside the experimental vessel (T, in Kelvin), and the volume of the sampling chamber (V, in liter). The equation also incorporates the volume of liquid ammonia (V_S, measured in microliters) and the molecular weight of ammonia (M, in g·mol^{-1}).

2.3 Data Processing method

As mentioned [15, 18, 19], the enose sensor response can be divided into three stages: the transient ascending stage, the overshoot stage, and the steady-state stage. While the transient ascent stage contains more information and data about the sensor response than the steady-state stage [20, 21], Figure 1 (a). displays the second-order response curve of the TGS and MQ gas sensors. In this experiment, both the data from the transient ascending stage and the steady-state stage were collected, processed, and analyzed as part of the dataset. Then, after using the sensor array to extract the gas characteristic information, MATLAB software is utilized for data processing, incorporating PCA and the construction of an ANN for enose data analysis in the Transient rise time area(A1) as well as steady-state(A2). These mentioned areas along with Both methods are investigated for different concentrations in terms of PPM and different odours.

2.3.1 Principal component analysis (PCA). PCA is a frequently utilized statistical method that can reduce the dimension of data and extract its characteristic information. With an increase in the number of sensors, the characteristic dimension of gas also increases [22].

2.3.2 Multilayer Perceptron (MLP). MLP is a type of Artificial Neural Network (ANN) that operates similarly to human neurons. It consists of an input layer, an output layer, and one or more hidden layers, with multiple neurons in each layer. The Figure 2 (a) shows a multilayer perceptron network topology assign for ammonia recognition at different concentrations using MQ37 and TGS813.

Table 2 illustrates that in mode 1, both areas have an input layer of 2, while the input layer for the second mode (M2) is set to 6. The output layer for all modes is set to 4, with 25 hidden layer neurons assigned. The proposed MLP structure utilizes the Rectified Linear Unit (ReLU) as the activation function (Equation 2), which enables MLP to perform nonlinear prediction and classification. This makes

Table 2: THE MLP Network Setting Over Different Mode, M1: Different Concentration (PPM), M2: Different Odor;

Mode	Area	Input layer(Neurons number)	Output layer(Neurons number)	Hidden layer(Neurons number)
M1	A1	2	4	25
	A2	2	4	25
M2	A1	6	4	25
	A2	6	4	25

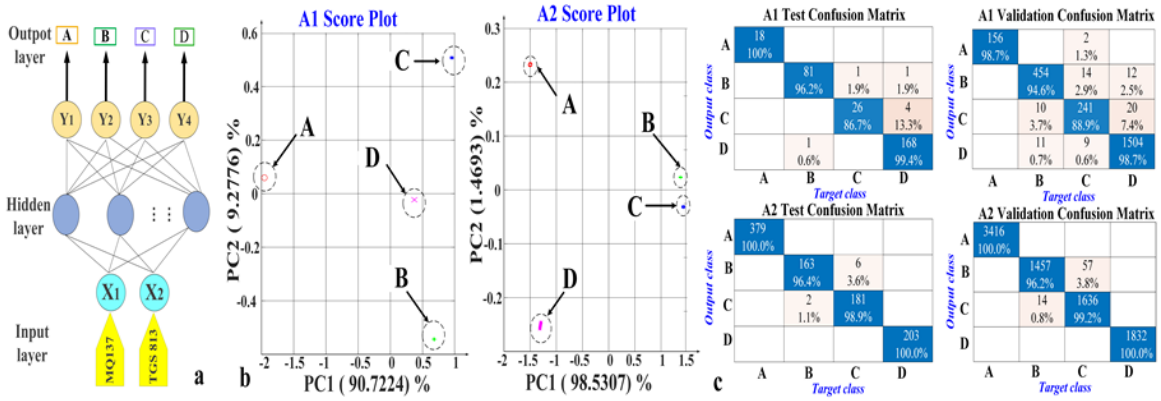

Figure 2: a: MLP network topology used; Results of four concentrations of ammonia b: PCA results and c: MLP results Ammonia concentration: A:100ppm B:200ppm C:400ppm D:AIR (0ppm)

it a useful tool for distinguishing and predicting gas types.

$$f(x) = max(0, x) \tag{2}$$

As Equation 2) shows if the input to the function (x) is greater than zero, then the output will be equal to x. If the input is less than or equal to zero, then the output will be zero. The ReLU function is popular in neural networks because it is computationally efficient and has been shown to produce good results in many different types of problems. Additionally, the ReLU function is easier to optimize using gradient-based methods, which are commonly used for training neural networks. One potential downside of the ReLU function is that it can "die" or "vanish" when the input to the function is negative, which can lead to problems with learning. In this paper, based on the proposed structure, the MLP networks for transient and steady-state phases are constructed, sensor data are used to train them respectively, and optimization models for different phases are obtained.

3 RESULT AND DISCUSSION

As mentioned before the data was collected and investigated in two areas of Transient rise time area (A1) and steady-state (A2) in two parts of Identification of different concentrations (PPM) of ammonia and odour identification which are described below.

3.1 Identification of different concentrations of ammonia

In this experiment, MQ137 and TGS813 sensors were used to collect data on four different concentrations of ammonia (100ppm, 200ppm, 400ppm, and pure Air). The steady-state stage contains a total of 9,346 data of MQ137 and TGS813 sensors, forming a matrix with a size of 9,346×2. The transient phase is 2,703 pieces of data. After normalizing the data, the PCA function is used to analyze the data. Using graph-related functions, score plots can be plotted to visually show the concentrations and types of gases.

The data used for MLP training was the same as that used for PCA, 10% of the data was reserved for testing the accuracy of the model, i.e. the data set used for training was an independent part of the whole data set. The parameters of the MLP model are shown in Table 2. The number of iterations is limited to 1000. The extracted data for both methods is shown in Figure 2. As the result shown in the PCA method for both A1 and A2 (transient response or the steady-state response), the sensors can distinguish gas of different concentrations from each other without concentrations overlapping. In both areas, indicating that the sensor array has a remarkable recognition effect on different concentrations of gas the PC1 is greater than 90%. By using the MLP method the classification of the steady-state stage (A2) by neural network is good, and the accuracy of discrimination of four concentrations is more than 95%, but the classification accuracy results in the transient-state stage (A1) are not as good as that in the steady-state stage around 88.9%. Besides the results shows, the resolution accuracy at 400ppm is less

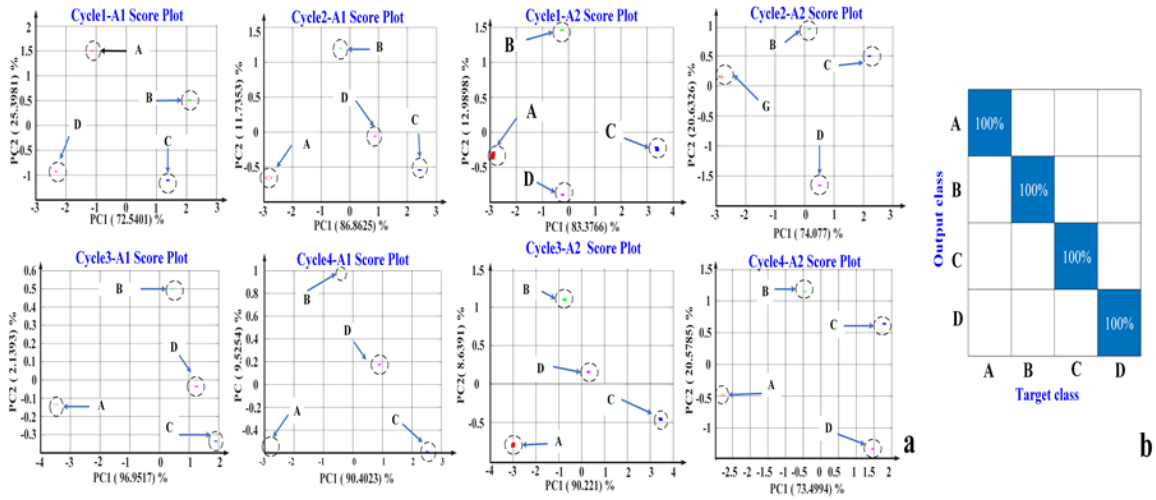

Figure 3: The obtained results in a: The PCA score chart of the transient stage(A1) and the steady-state stage(A2), b: MLP classification confusion matrix. A: Air1 (a mixture of air and Ethanol) B:ammonia (pure ammonia gas) C: Air 2(a mixture of air and Ammonia) D: ethanol (pure ethanol gas)

Table 3: The odour Identification over PCA and MLP, A1: Transient rise time area A2: Steady-state stage area

Method/ Area	Parameter		Cycle1	Cycle2	Cycle3	Cycle4
PCA-A1	PC1		72.51%	86.86%	96.95%	90.40%
PCA-A2	PC1		83.38%	74.08%	90.22%	73.50%
MLP-A1	Training	data volume	159	185	159	197
		Accuracy	100%	100%	100%	100%
	Test	data volume	17	20	17	21
		Accuracy	100%	100%	100%	100%
MLP-A2	Training	data volume	720	360	360	360
		Accuracy	100%	100%	100%	100%
	Test	data volume	80	40	40	40
		Accuracy	100%	100%	100%	100%

than 90%, against the resolution accuracy at other concentrations with 95%.

3.2 Different Odour Identification

As the second result to detect the different odours, a sensor array changed, and use the MQ2, MQ3, MQ5, MQ6, MQ7, and MQ137 sensors are used to identify four kinds of gases with gas concentrations of 200ppm. considering the odour the four types of gas with the fixed ppm values are used as follows; Air1 (a mixture of air and Ethanol), Air 2(a mixture of air and Ammonia), ethanol (pure ethanol gas), and ammonia (pure ammonia gas); A complete data acquisition cycle of the sensor includes the transient response stage and the steady-state response stage. The experiment is carried out four times with four cycles. At the end of each cycle, fans and air pumps are used to ventilate the sampling room and exhaust the sampling room. PCA and MLP were used to analyze the more than 10,000 samples of data in the experiment. 10% of the data was reserved for testing the accuracy of the model, The obtained results are shown in Figure 3 and Table 3.

As the result shows, PCA score plots of steady-state and transient-stage under four cycles of data acquisition, all gas types are distinguished from each other in pairs, and the sensor array can distinguish different types of gas. Detailed results of PCA and MLP are shown in Table 3.

The accuracy of PCA in identifying the four gases is not as good as the accuracy in identifying the four ammonia concentrations. However, PC1 is greater than 70%, which can effectively distinguish the types of gas. The recognition accuracy of MLP is 100%, and the recognition effect is very excellent. In general, the accuracy of PCA is not as high as MLP in the identification of the four gases.

4 CONCLUSION

Detecting ammonia gas is critical for a variety of reasons, including protecting occupational safety by identifying this toxic gas and its impact on human health, monitoring ammonia as an environmental

pollutant, and ensuring food safety by detecting its use in refrigeration and the production of certain foods, such as baked goods and chocolate. Studying gas sensor response in both transient and steady-state regions offer numerous benefits. Figure 1 illustrates that data collected during the transient response period, which typically lasts around 20 seconds, is much faster than the 40 seconds required during the steady-state response phase. This delay allows the sensor response to stabilize, resulting in a 50% reduction in sensor performance time when operating in the transient region. This study utilized MQ and TGS series semiconductor sensors to construct an electronic nose system sensor array. By analyzing data with PCA and MLP neural networks, the researchers discovered that the electronic nose system could differentiate various concentrations of ammonia in both the steady-state and transient response stages, as well as distinguish ammonia from other gases. The MLP was successful in distinguishing gas concentrations except for concentrations exceeding 200 ppm and 400 ppm. The sensor array demonstrated the ability to work in both transient and steady-state response phases, and data could be read without the need to enter a steady state, resulting in significant time savings. However, the accuracy of estimating transient gas concentration may be compromised due to various reasons. For instance, the insufficient training data with fewer data points for transient analysis as compared to steady-state analysis, rapid changes, and shorter duration of the transient phase, and concentration identification sensor array consisting of only two sensors may fail to produce significant differences in sensor responses at similar high concentrations such as 200ppm and 400ppm. Future work will entail investigating additional machine learning methods to analyze and study sensor response, exploring the performance of E-nose in steady-state and transient time while examining the impact of temperature and humidity.

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